

Monte Carlo Simulation of Homopolymer Melts in Plane Poiseuille flow

J.R. Dorgan and S.S. Gleiman
Department of Chemical Engineering
Colorado School of Mines
Golden, CO 80401 U.S.A.

A special biased Monte Carlo algorithm is used to study flow of homopolymer melts between neutral, hard walls on a fcc lattice at full occupancy ($\phi = 1$). A random number biasing technique is developed to mimic slot flow of a melt; the biasing method preferentially moves the chains in the direction of flow. System properties including velocity profiles, chain-end density distributions, average radii of gyration, and end-to-end vector order parameters are investigated as functions of chain length and biasing parameter. Chain connectivity leads to non-Newtonian flow behavior evidenced as velocity profile blunting. Observations suggest a relationship between the logarithm of the biasing parameter and the pressure drop. Based on the prescribed biasing profile, it is shown that flow causes greater chain deformation for longer chains ($N = 64, 128$) than for smaller chains ($N = 16$). Findings also include the ordering of chains with end-to-end vectors aligned with respect to the flow direction.